Development and Validation of a Simulation Tool to Predict the Combined Structural, Electrical, Electrochemical, and Thermal Responses of Automotive Batteries

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Ford Motor Company

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Jun 6, 2017

Project ID – ES296

Overview

Timeline

- Start: Jan 1, 2016.
- End: Dec 31, 2018.
- Percent completion: 42%.

Barriers Addressed

- Battery/Energy Storage R&D
  - Cost.
  - Abuse tolerance.
    - Robust to the safety requirements.

Budget

- Total contract value: $4.375M
  - $3.5M DOE/TARDEC share
  - $875k Ford share
- Funding received in 2016: $695k (EERE)
- Funding for FY 2017: $1.187M (EERE)

Subcontracts

- Project lead: Ford Motor Company.
- Subcontractor: Oak Ridge National Laboratory (ORNL).

Relevance

- **Project objective**: Develop a simulation tool to predict the combined structural, electrical, electrochemical, and thermal (EET) responses of automotive batteries to crash-induced crush and short circuit, overcharge, and thermal ramp and validate it for conditions relevant to automotive crash.

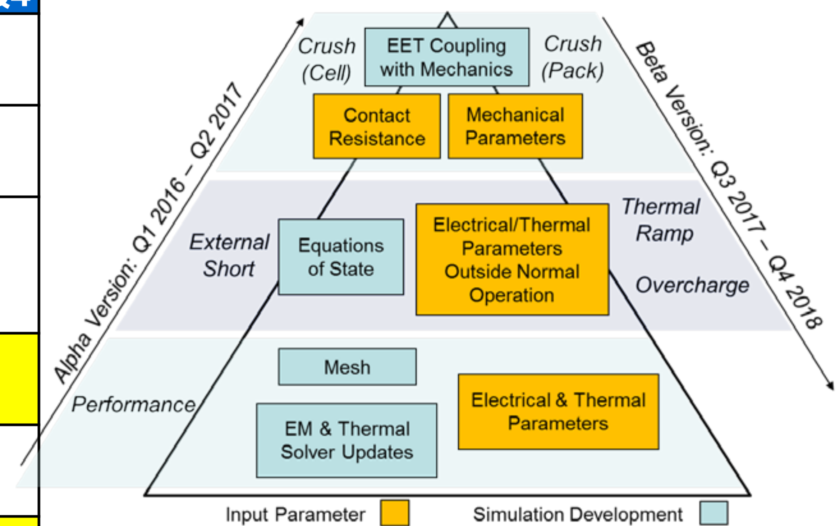
- **Impact**:
  - Cost.
    - Cost reduction by shortening development cycle and optimizing crash protection systems.
  - Abuse tolerance performance.
    - Improvement in abuse tolerance by delivering a predictive simulation tool to shorten or eliminate design – build – test prototype cycles and accelerating development and optimization of crash protection systems robust to the safety requirements.

Milestones

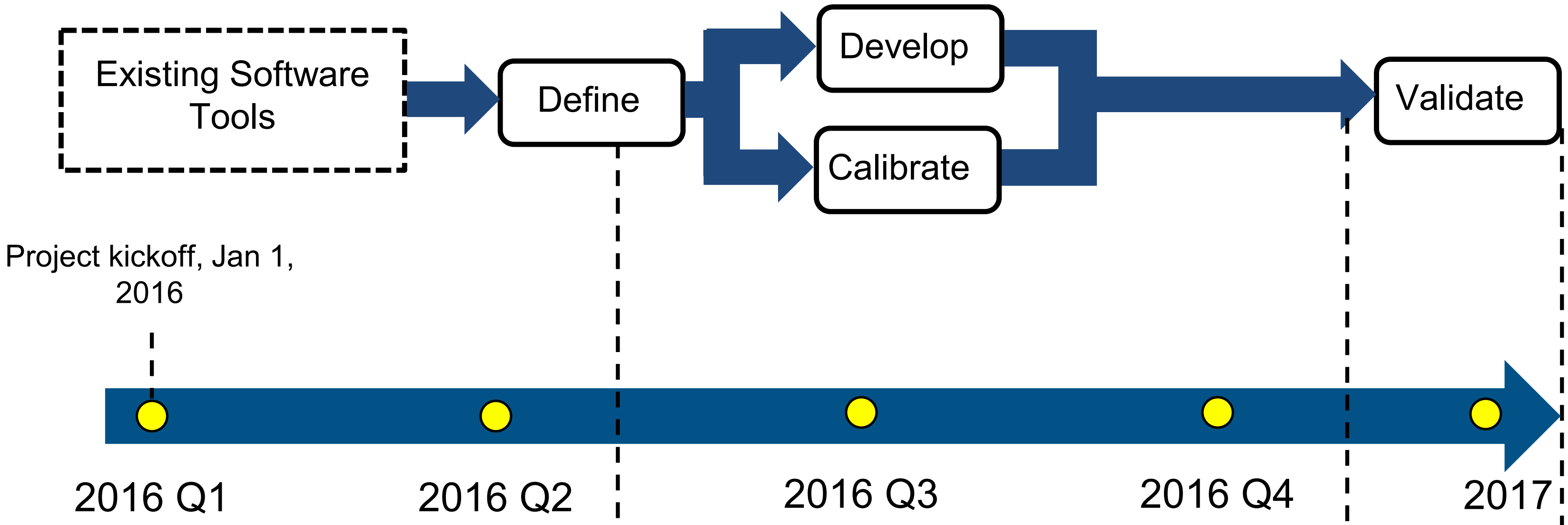
Tasks	2016				2017			
	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
Hardware selection for Alpha version								
Development assumptions for Alpha version								
Alpha version multi-physics solvers and material models (75%)								
Alpha version model inputs (60%)								
Integrate solvers into Alpha version (33%)								
Validation of Alpha version (30%)								
Development assumptions for Beta version								
Hardware selection for Beta version								
Beta version multi-physics solvers and material models								

Not started　On-track　Complete

Project Plan



Approach – Model Development



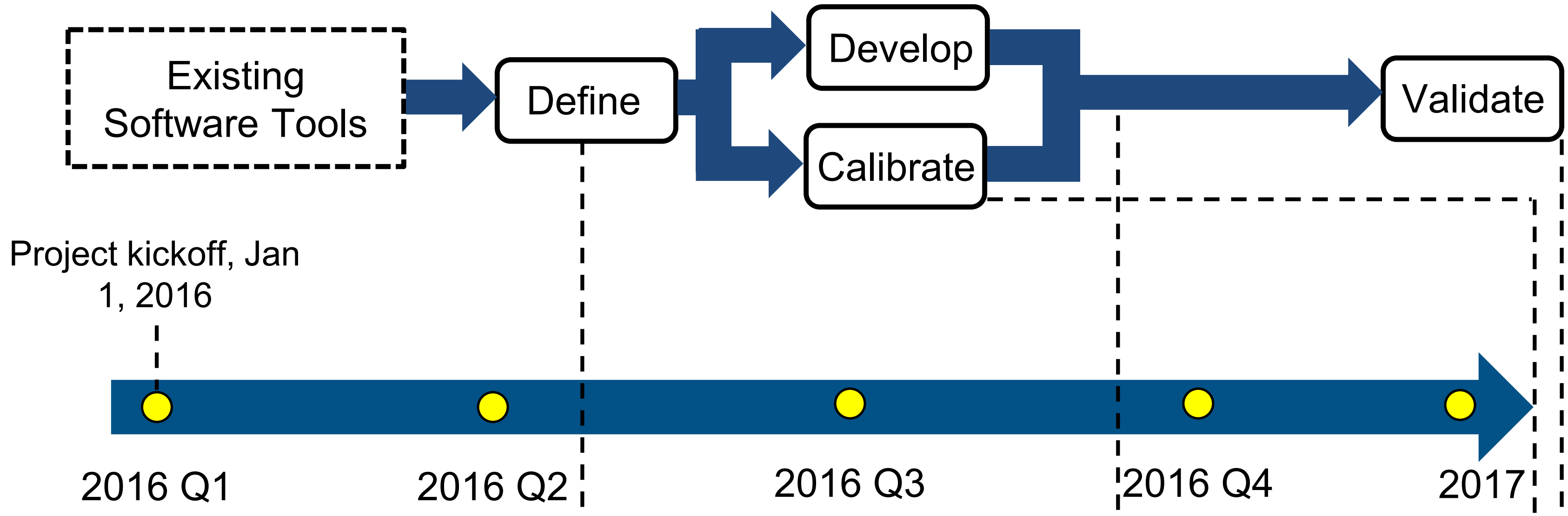
M2: Benchmarking analysis of existing models completed. Consider computational requirements, model robustness for typical case studies, and required inputs.
M3: Formulate development assumptions for solver enhancements. Target advancements that significantly reduce computational requirements and improve robustness beyond existing models.

DP1: Demonstrate preliminary version of CAE software for cell-level crush multi-physics response, prior to full-scale validation.

M6: Complete multi-physics solvers and material models.
M7: Integrate solvers into Alpha version model. Update user-interfaces for pre/post processing.

Not started | On-track | Complete

Approach – Model Validation



M1: Select hardware for model validation activities. Choose cell formats and chemistries that are broadly applicable to the automotive market, with particular emphasis on high-energy cells.

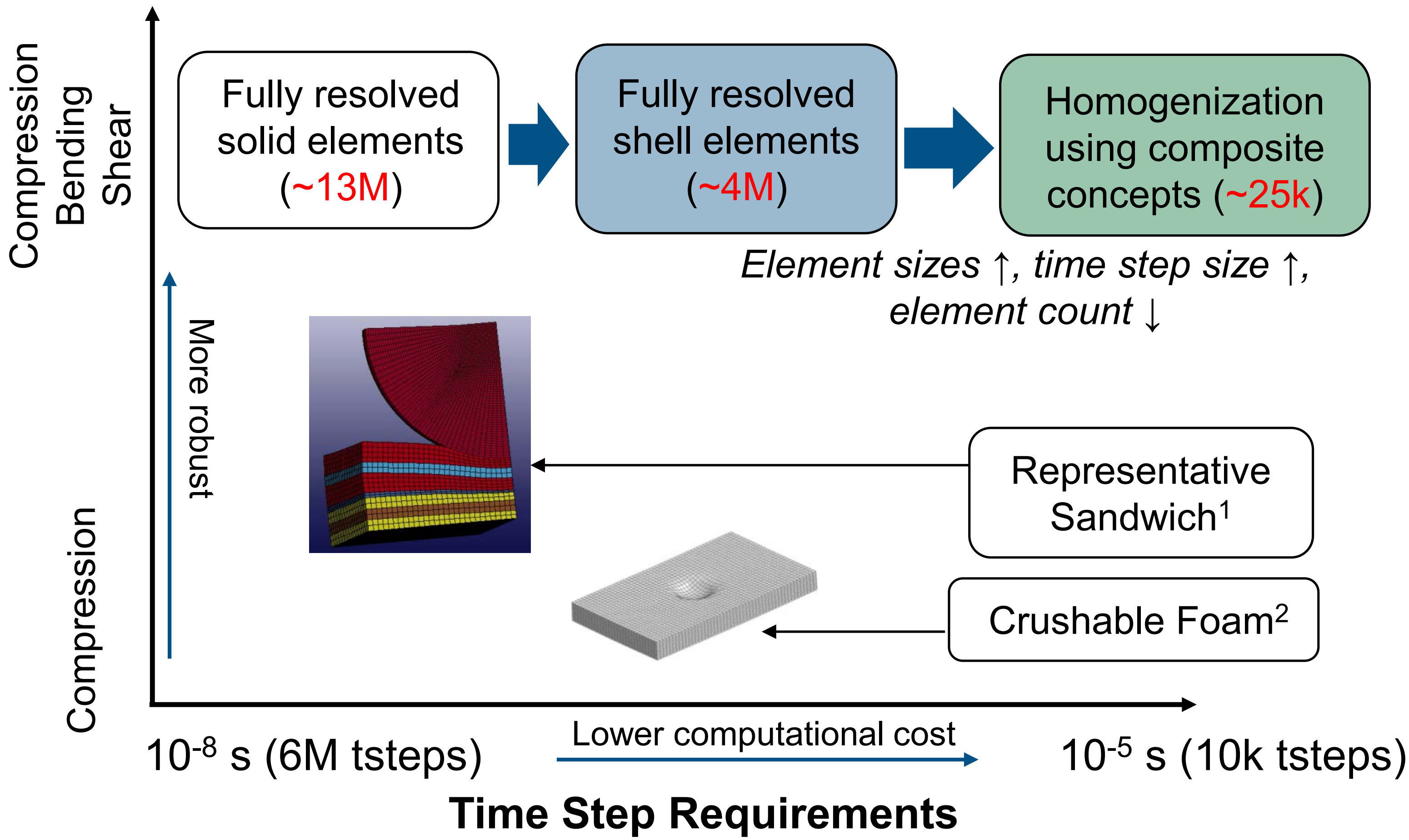
M4: Identify test site and define validation tests. Validation will primarily consist of high strain rate impact testing in a variety of orientations and energy levels.

DP2: Cell-level validation of simulation tool completed for full range of mechanical testing.

M5: Complete database of model inputs for model validation activities, including electrical, electrochemical, thermal, and mechanical inputs.

Not started | On-track | Complete

Approach – Targeted Development

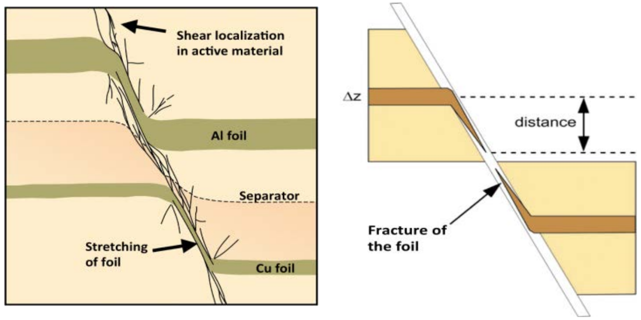


Key: Ford Lead | ORNL Lead | Literature Approach | Element Count

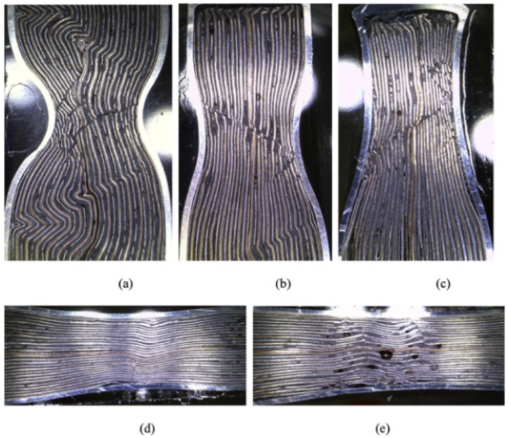
1) J. Power Sources, 290, 102 – 113 (2015). 2) J. Power Sources, 201, 307 – 321 (2012).

Technical Accomplishments and Progress: Development of Layered Solid Model (ORNL)

- Failure mechanism.
  - Initial homogeneous compression of the J/R.
  - Increased loading exceeds the strength of the J/R resulting in a localized fault formation.
  - Materials flow and internal rearrangement.
  - Separator failure leading to internal short circuit as opposite electrode materials come into contact.

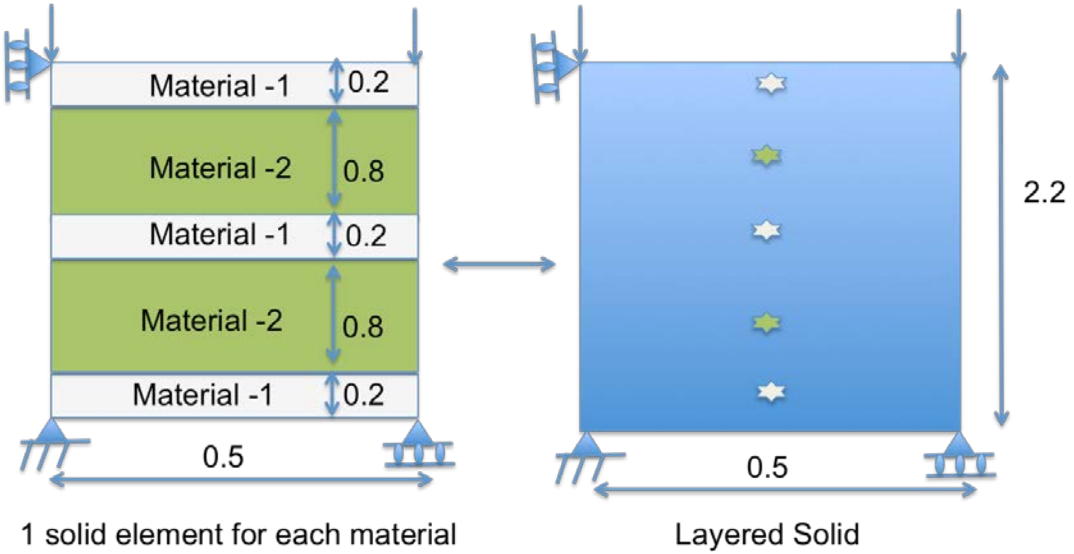


- Approach for modeling of cell deformation (Layered solid).
  - Avoid modeling of every layer and interface with separate finite elements.
  - Multiple layers in a single finite element allow for modeling of cooperative faults, interfacial faults, between the layers, while scaling up the cell response.
  - Faster than solid element model.



Technical Accomplishments and Progress: Development of Layered Solid Model –Through Thickness Compression

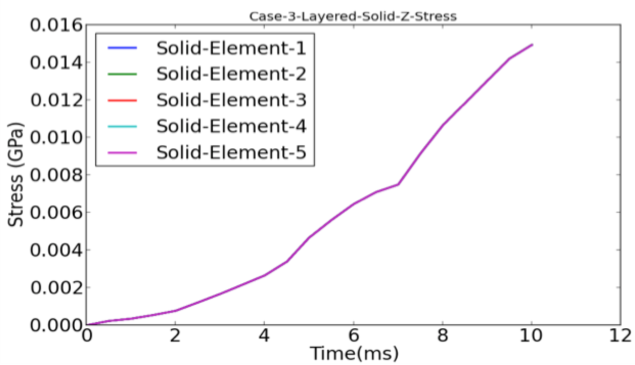
- The objective is to have response of the solid element assembly be the same as for the single layered element with integration points located in the corresponding layer locations.
- Employed is commonly used material models for electrode materials.
- Crushable Foam (MAT-63) and Elasto-Plasticity (MAT-24) for current collector and separator.
  - Material 1 → MAT – 24 & Material 2 → MAT – 63.

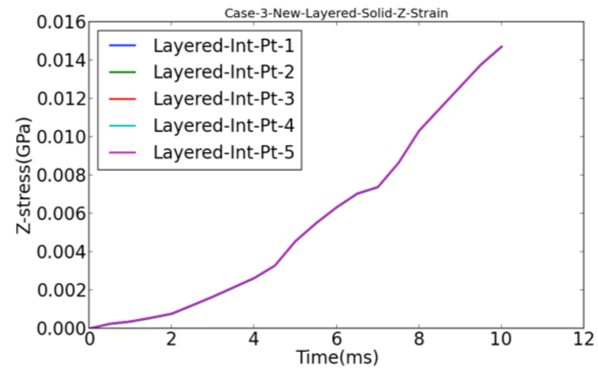


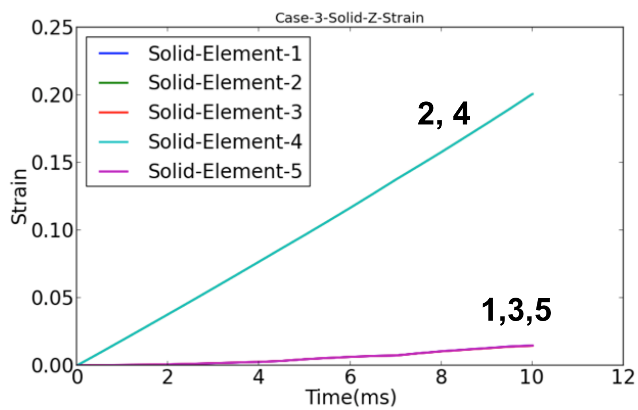
<u>**Fully Resolved** (1 solid element for each material)</u>
- # elements = 5
- Minimum element thickness = 0.2

<u>**Layered Solid**</u>
- # elements = 1
- Minimum element thickness = 2.2

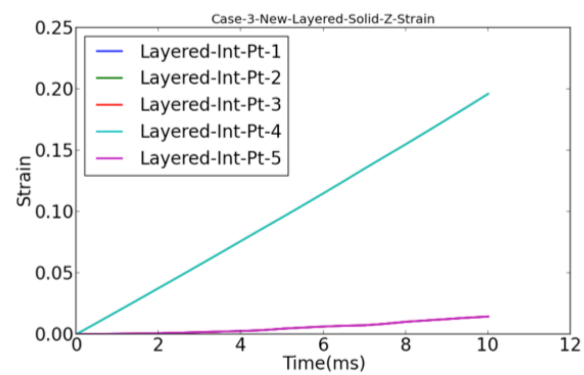
Technical Accomplishments and Progress: Layered Solid Model –Through Thickness Compression Simulation Results







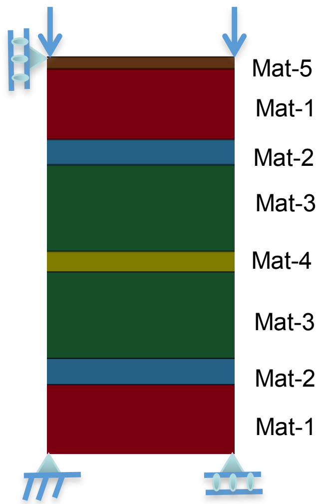
Solid Element



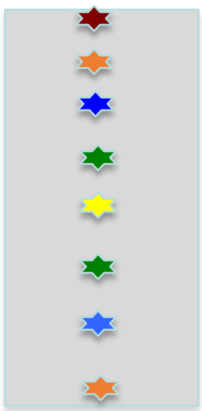
Layered Solid

- The new layered solid element formulation in LS-DYNA gives the same response as the assembly of solid elements.
- The new layered solid element formulation reduces the number of degrees of freedom, computational time, and account for the cell inhomogeneity.

Technical Accomplishments and Progress: Layered Solid Model – Multi Material Configuration Test



Solid element assembly

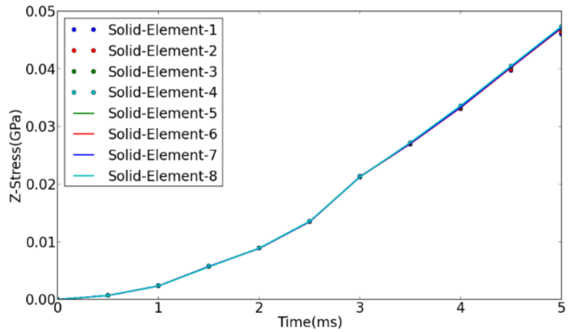


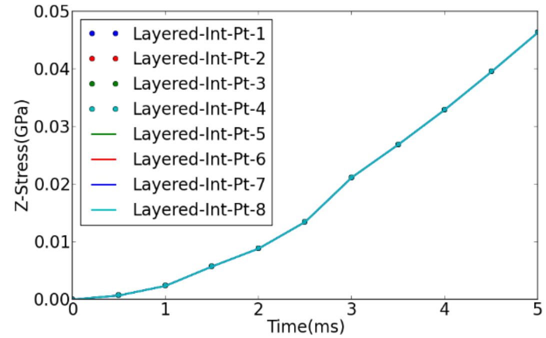
Layered solid element

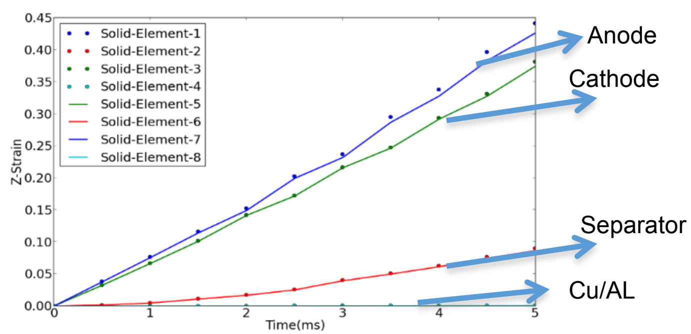
Component	Material	Material Model	Thickness (mm)	Elastic Modulus (GPa)
Anode	Mat-1	Mat-63	0.065	0.465
Separator	Mat-2	Mat-24	0.024	0.5
Cathode	Mat-3	Mat-63	0.080	0.55
Aluminum	Mat-4	Mat-24	0.019	70
Copper	Mat-5	Mat-24	0.011	110

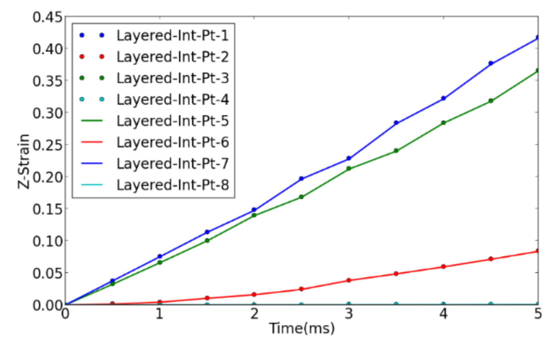
- Test of new formation for material properties are characteristic of a cell J/R.
- Notice large contrast in properties of different layers.
- In assemblies of solid elements without constraints, such contrast would lead to large numerical instabilities.

Technical Accomplishments and Progress: Layered Solid Model – Multi Material Configuration Test Results





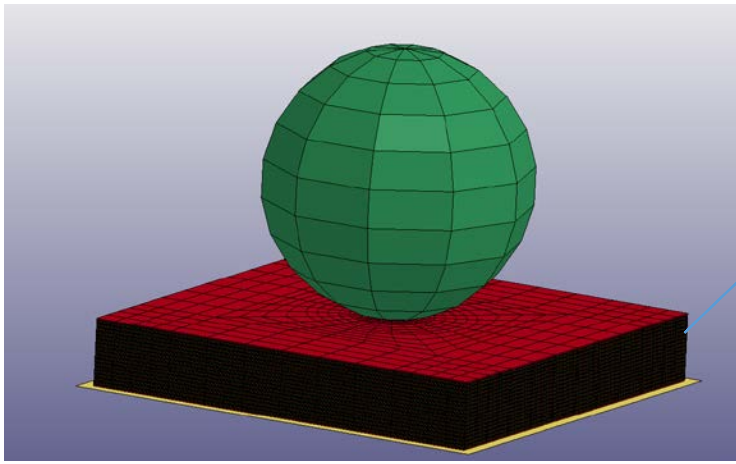


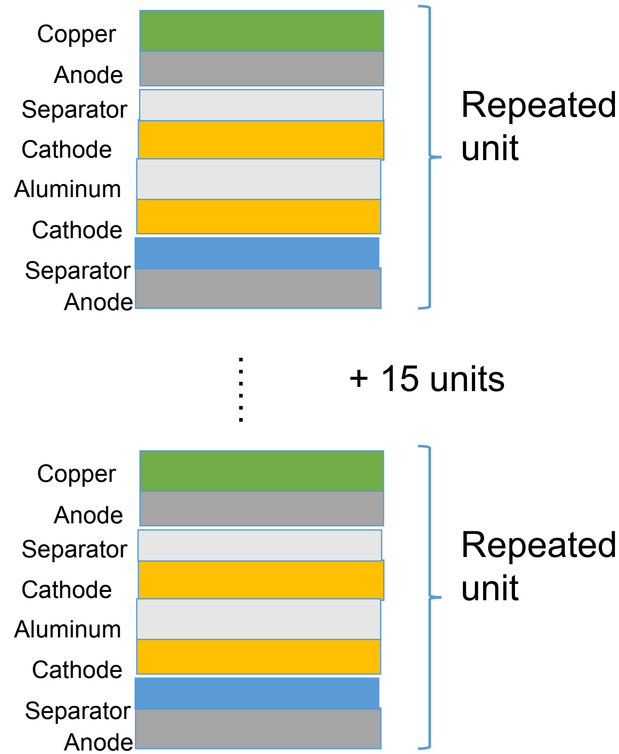


Solid Elements **Layered Solid**

- Responses are the same even for large contrasts in material types and properties.
- One layered element replaces 8 solid elements.

Technical Accomplishments and Progress: Layered Solid Model – Cell Indentation_Solid Elements



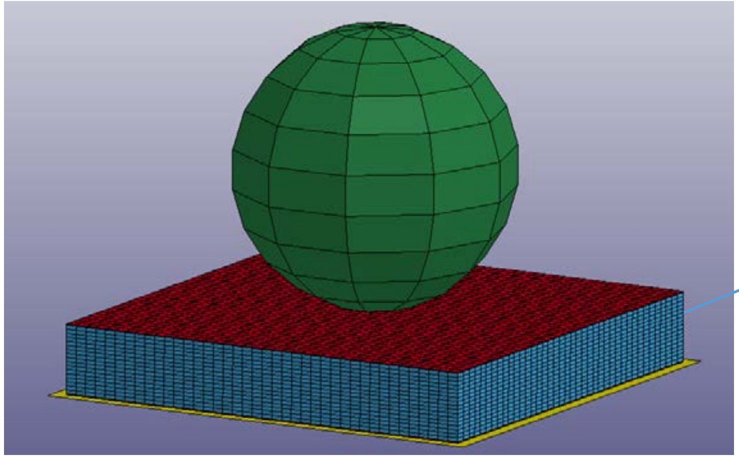


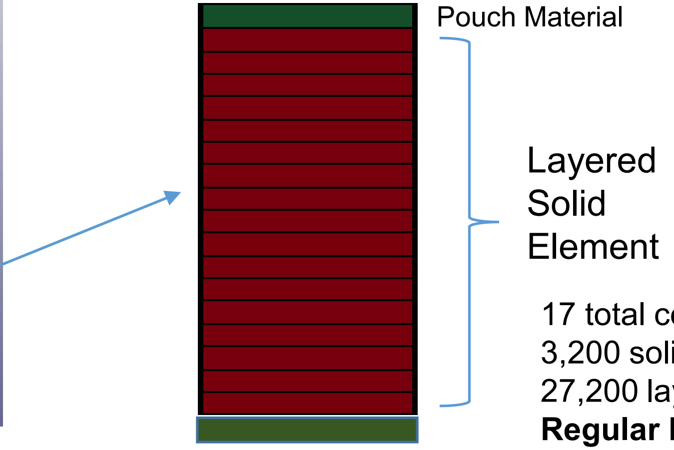
Component	Thickness (mm)	Material Model	Elastic Modulus (GPa)	Yield Strength (GPa)
Copper	0.011	MAT-24	110	0.24
Anode	0.064	MAT-24	0.45	0.04
Separator	0.024	MAT-24	0.5	0.06
Cathode	0.080	MAT-24	0.55	0.04
Aluminum	0.018	MAT-24	70	0.24

2 pouch layers at the top and bottom
17 total cell layers
556 elements per layer
76,728 solid elements

Gradient mesh was necessary to control the size of the model.

Technical Accomplishments and Progress: Layered Solid Model – Cell Indentation_Layered Solid Elements

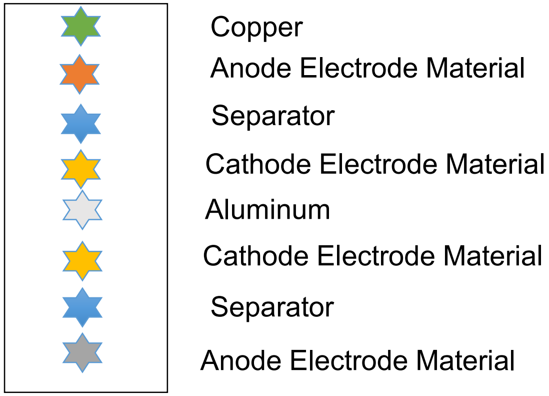




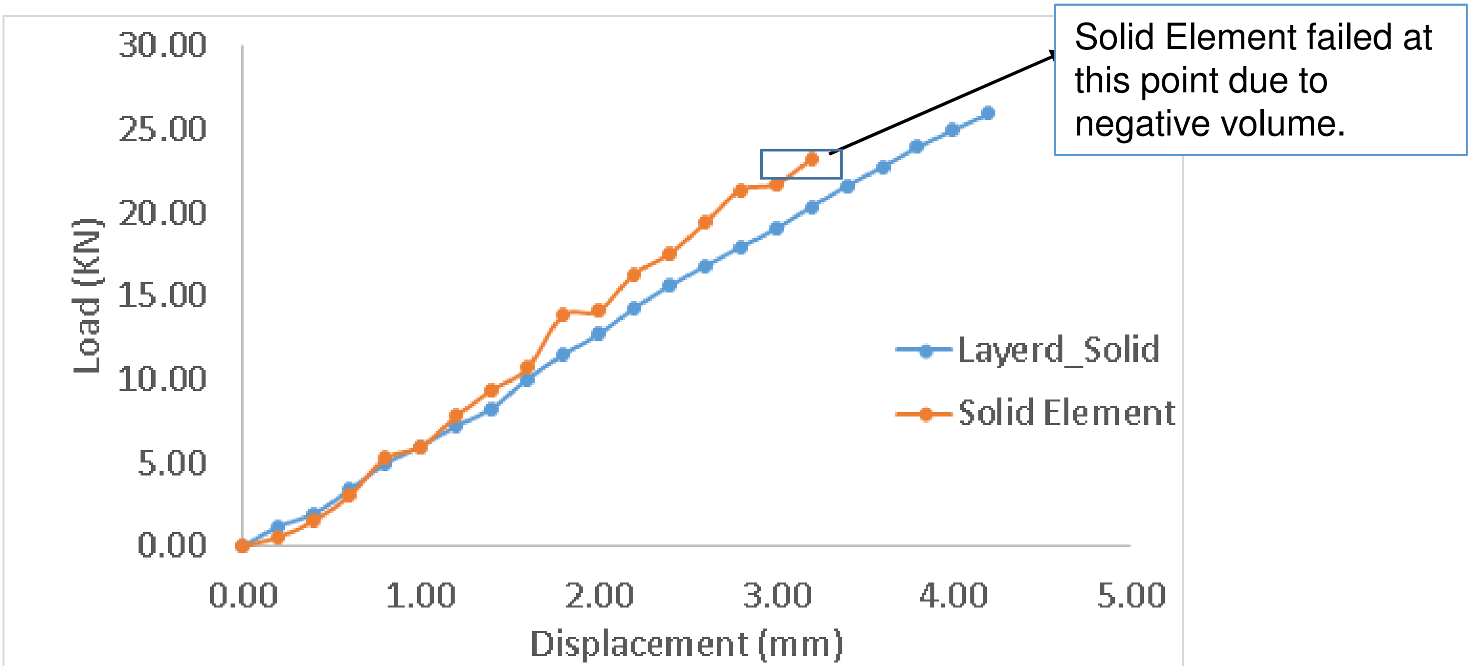
17 total cell layers
3,200 solid elements (pouch)
27,200 layered solid (cell)
Regular Mesh

Component	Thickness (mm)	Material Model	Elastic Modulus (GPa)	Yield Strength (GPa)
Copper	0.011	MAT-24	110	0.24
Anode	0.064	MAT-24	0.45	0.04
Separator	0.024	MAT-24	0.5	0.06
Cathode	0.080	MAT-24	0.55	0.04
Aluminum	0.018	MAT-24	70	0.24

Layered Element

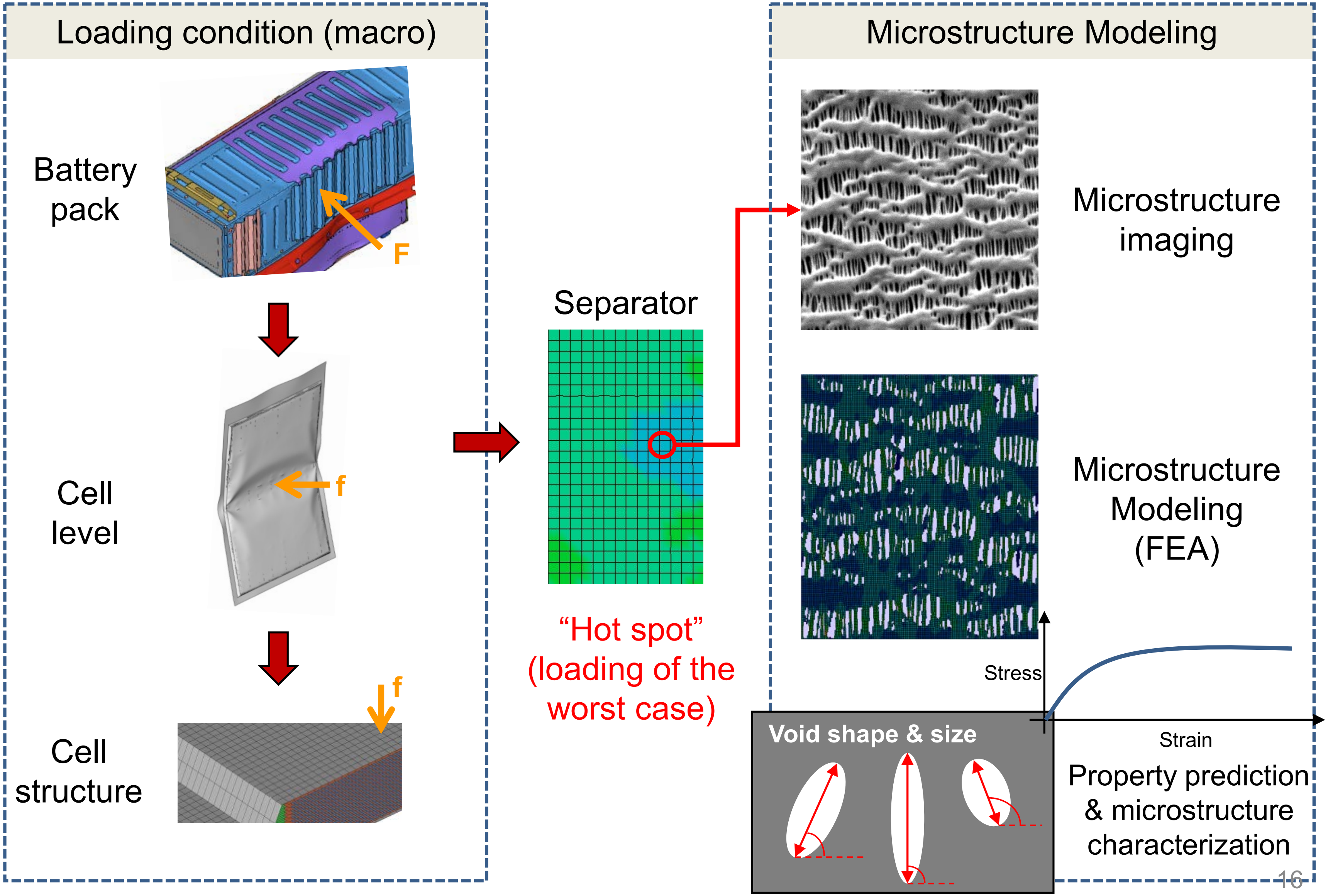


Technical Accomplishments and Progress: Layered Solid Model – Indentation Simulation Comparison

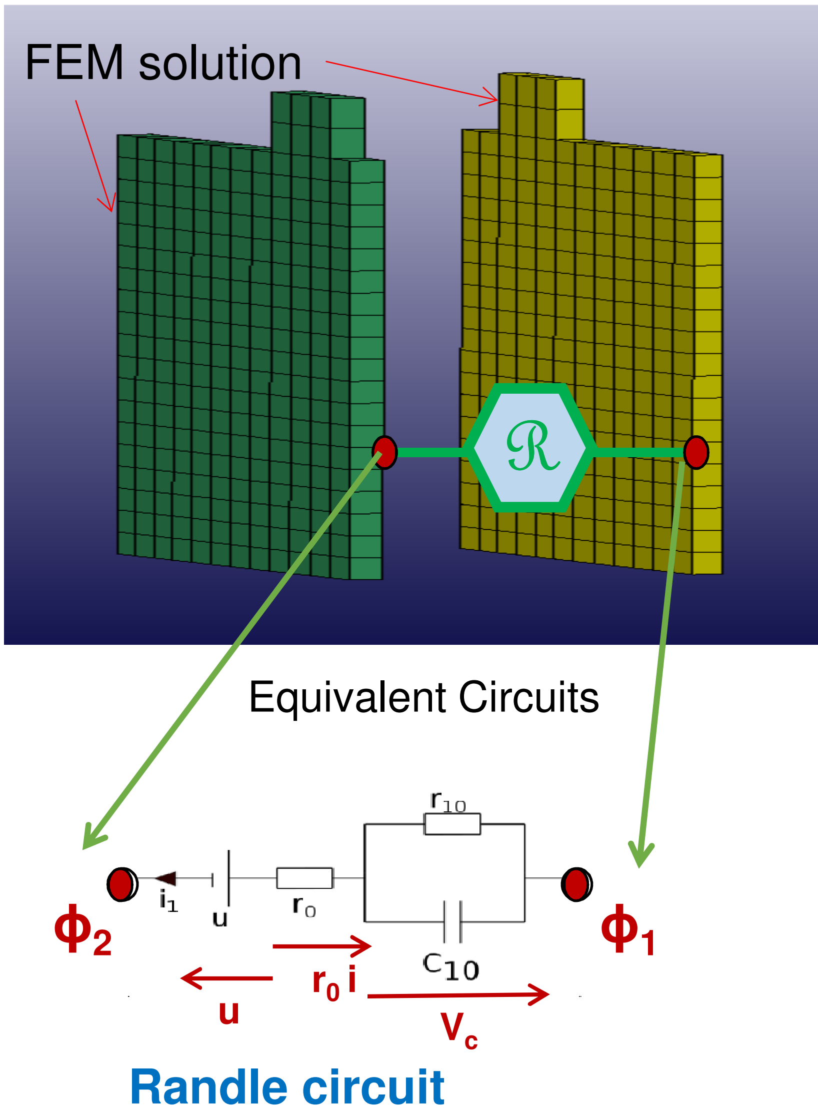


- Solid element CPU time = 52,705 sec.
- Layered solid element CPU Time = 2,248 sec.
- New layered element formulation is **22.8** times faster while having **2.52** times fewer elements.

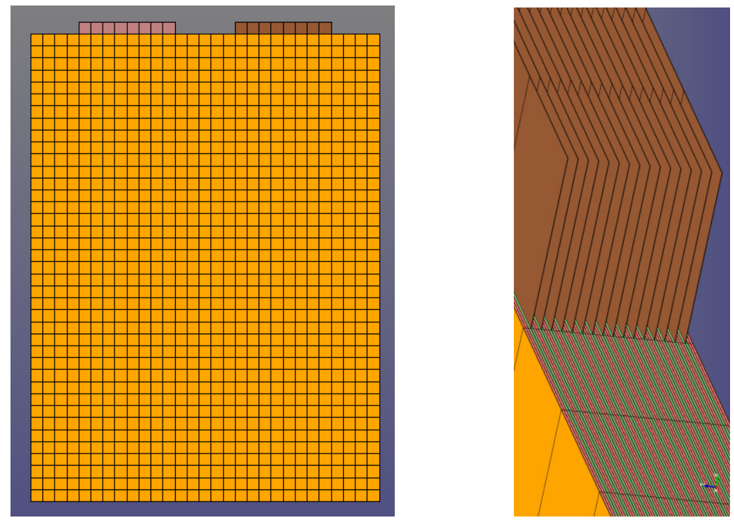
Technical Accomplishments and Progress: Microstructure Model (Ford)



Technical Accomplishments and Progress: LS-DYNA EM Resistive Solver & Electrical Model Development Progress



Current Mesh Implementation



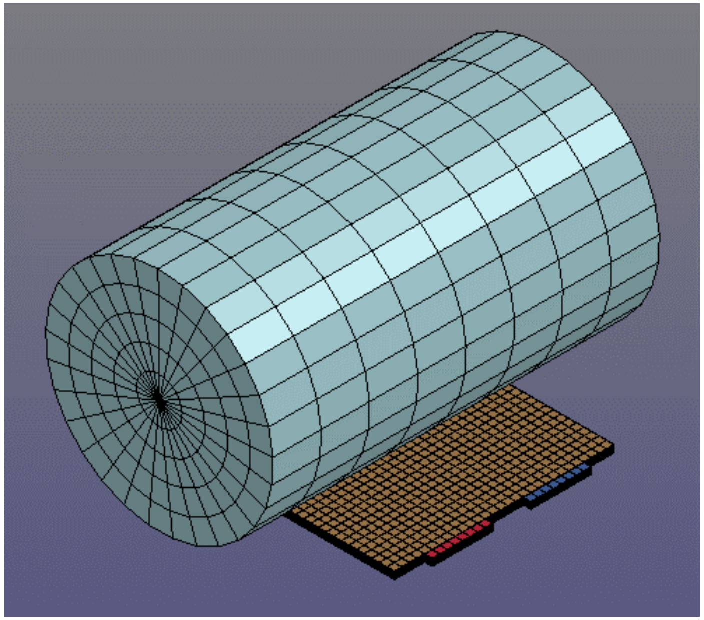
- 5 mm edge length
- ~150k elements per cell
- 1 element per component thickness

Model Inputs

- Bulk heat capacity and thermal conductivity
- Cell-level calibration of circuit parameters
- Type A cell (15 Ah pouch, Graphite & NMC/LMO)

Technical Accomplishments and Progress: Internal Short Model – Cell Crush Model Set Up

Simulation Mesh



Experimental Setup

Target Time Steps

Crash
(Vz = 5 m/s)

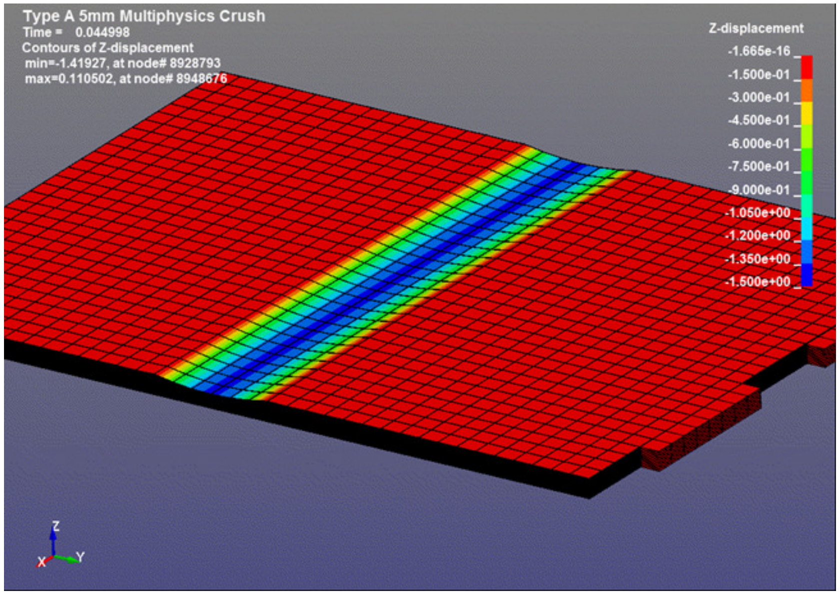
Mech + Electrical + Thermal
tf = 0.2 ms; dt = 0.2 μs

"Freeze" mechanics

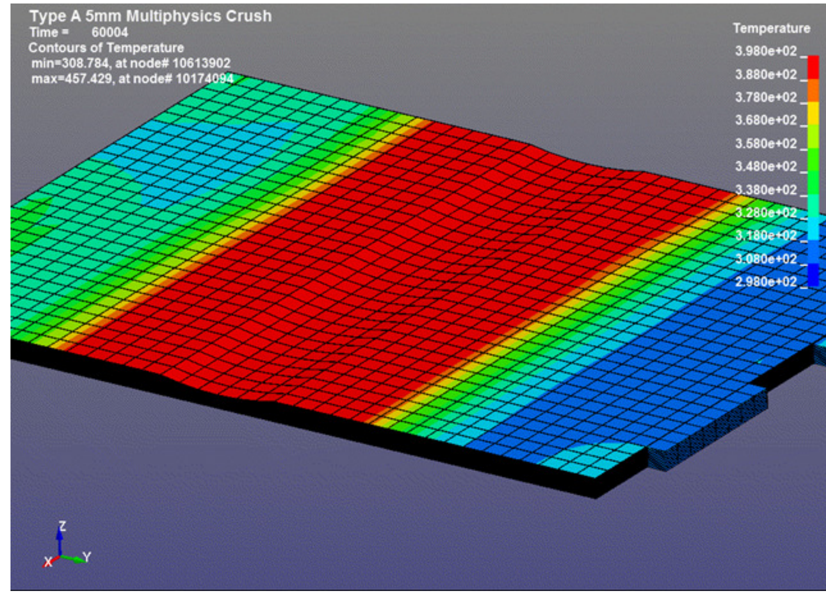
Electrical + Thermal
tf = 50 s; dt = 1 s

Technical Accomplishments and Progress: Crush Coupling with Multi-Physics Solvers

Nodal Z-Displacement



Thermal Fringe Plots

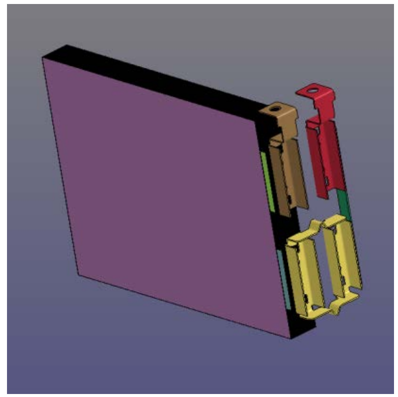


- Coupling with multiphysics using deformable to rigid switch for "crash" case study and newly developed LS-DYNA keyword *EM_RANDLE_SHORT.
- Assuming compressive strain causes onset of short circuit.
- Future work will focus on accuracy and robustness improvements, and integration with ORNL layered solid models.

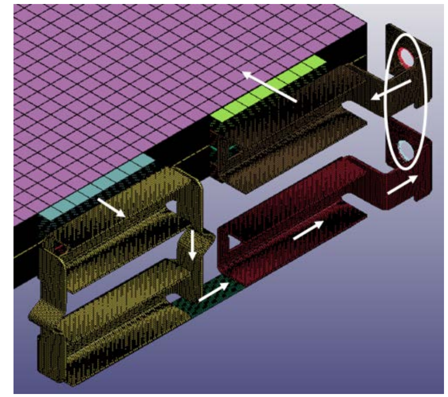
Technical Accomplishments and Progress: External Short Model

Test Hardware

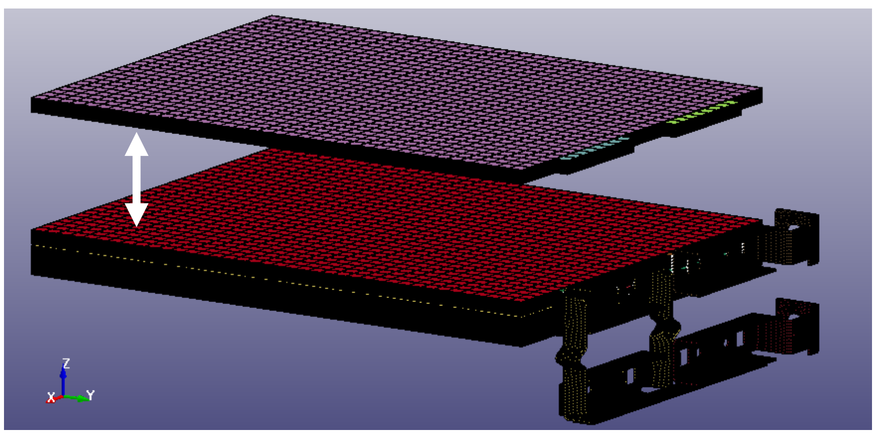
Simulation Mesh



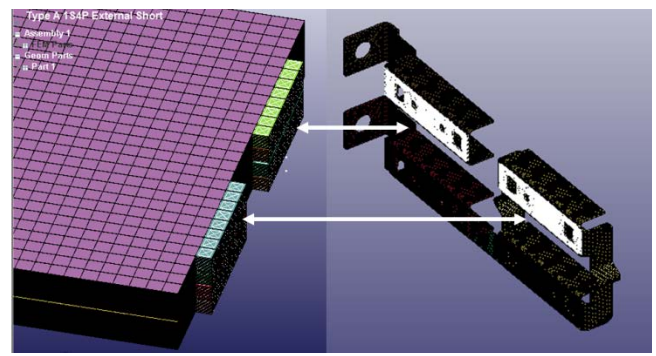
Current Pathway



Cell-to-Cell Heat Transfer



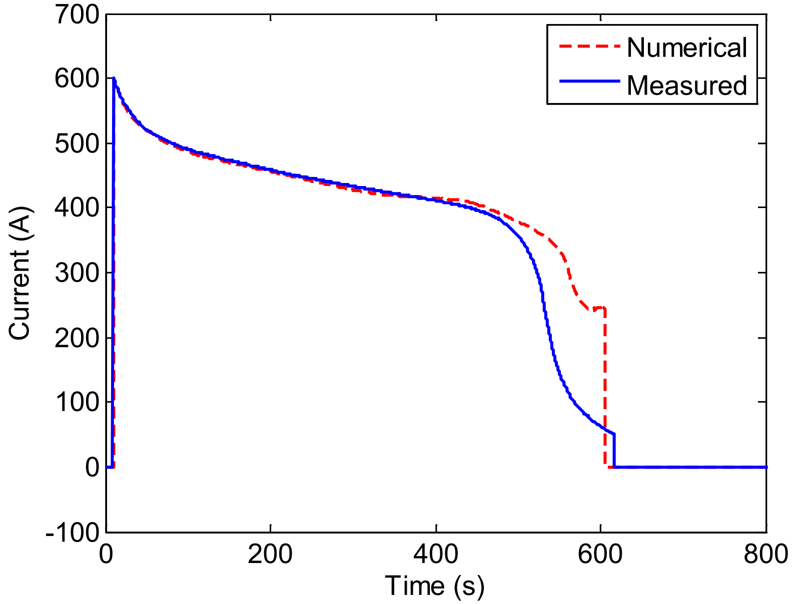
Cell-to-Bus Thermal and Electrical



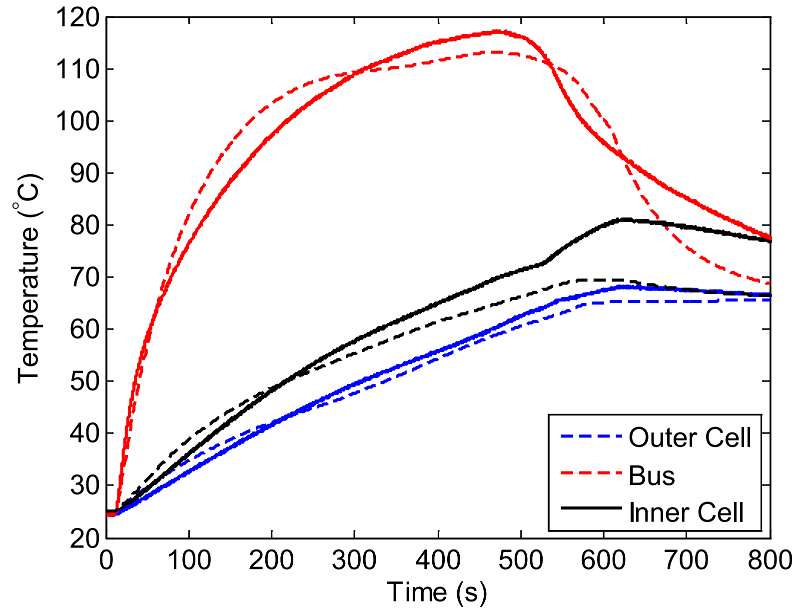
- *Leveraging our legacy experiments to confirm model developments prior to full-scale validation*
- *Simulation set up to match a DOT/NHTSA project Type A 1S4P module external short circuit using newly developed LS-DYNA keywords *EM_RANDLE and *EM_ISOPOTENTIAL*

Technical Accomplishments and Progress: External Short Circuit Validation

Model Predicted Current versus Experiment



Model Predicted (Dashed) Temperatures versus Experiment (Solid)

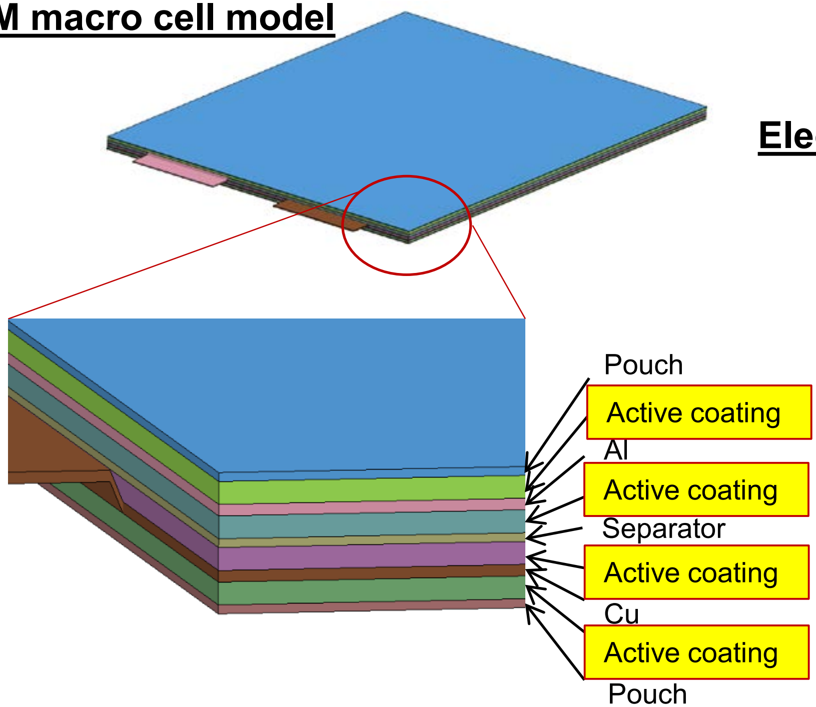


- Good agreement between numerical and measured data for electrical variables.
- Thermal predictions demonstrate agreement of 5-10 °C between numerical and experimental data (excluding >550 s for inner cell).

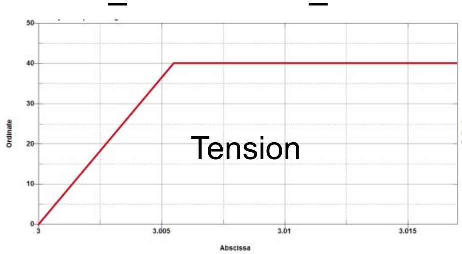
Technical Accomplishments and Progress: Mechanical and EM Simulation of Module (5P4S)

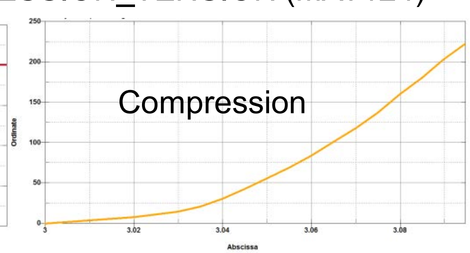
- Objectives
  - Simulate mechanics to define electrical contact points.
  - Simulate external short circuit EM and thermal response.

EM macro cell model

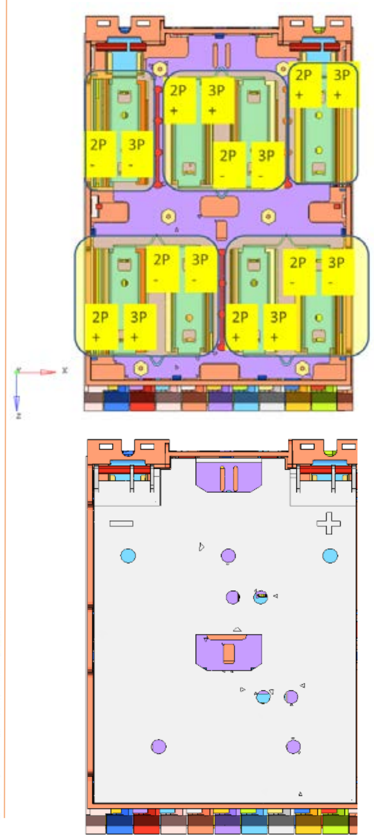


Active coating:
*MAT_PLASTICITY_COMPRESSION_TENSION (MAT124)

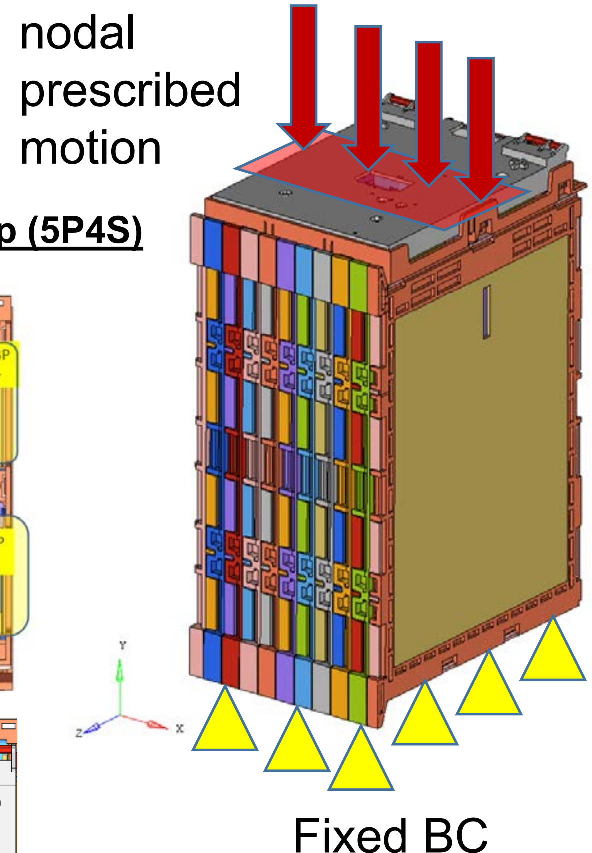




Electrical connection setup (5P4S)



Module crush CAE run setup

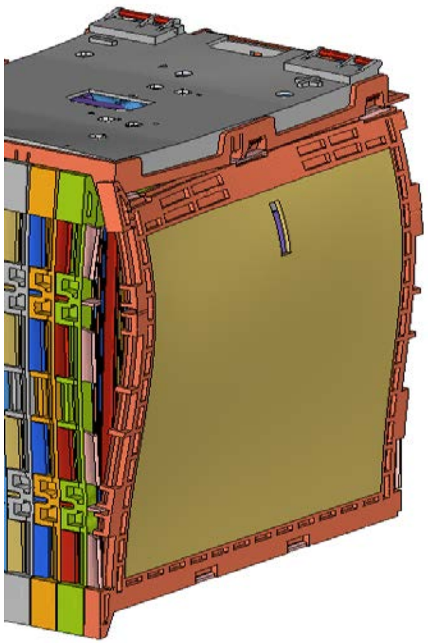


Technical Accomplishments and Progress: Mechanical and EM Simulation of Module – Crush Results

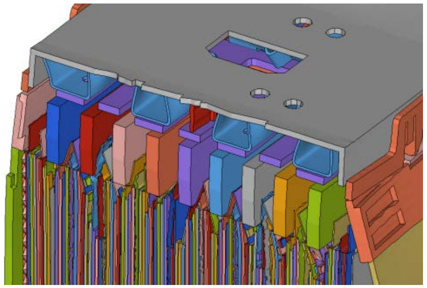
- Crush CAE results

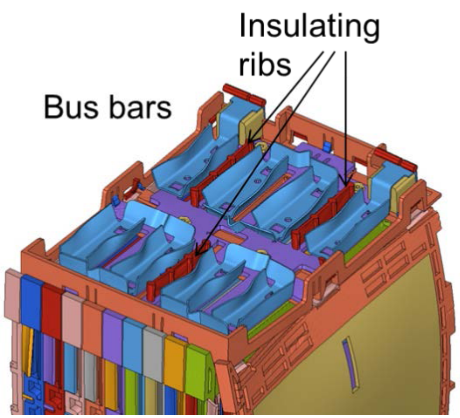
Deformation

@ 5mm in crush amount

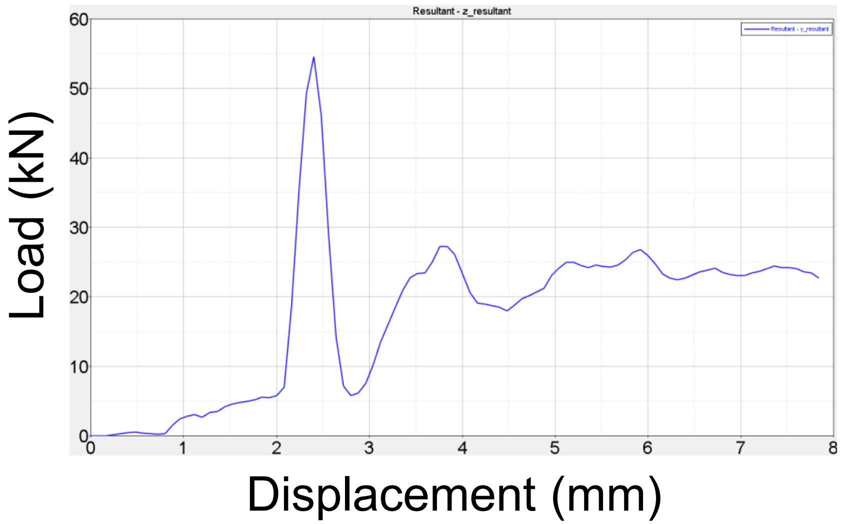


Cell tabs





Force-displacement

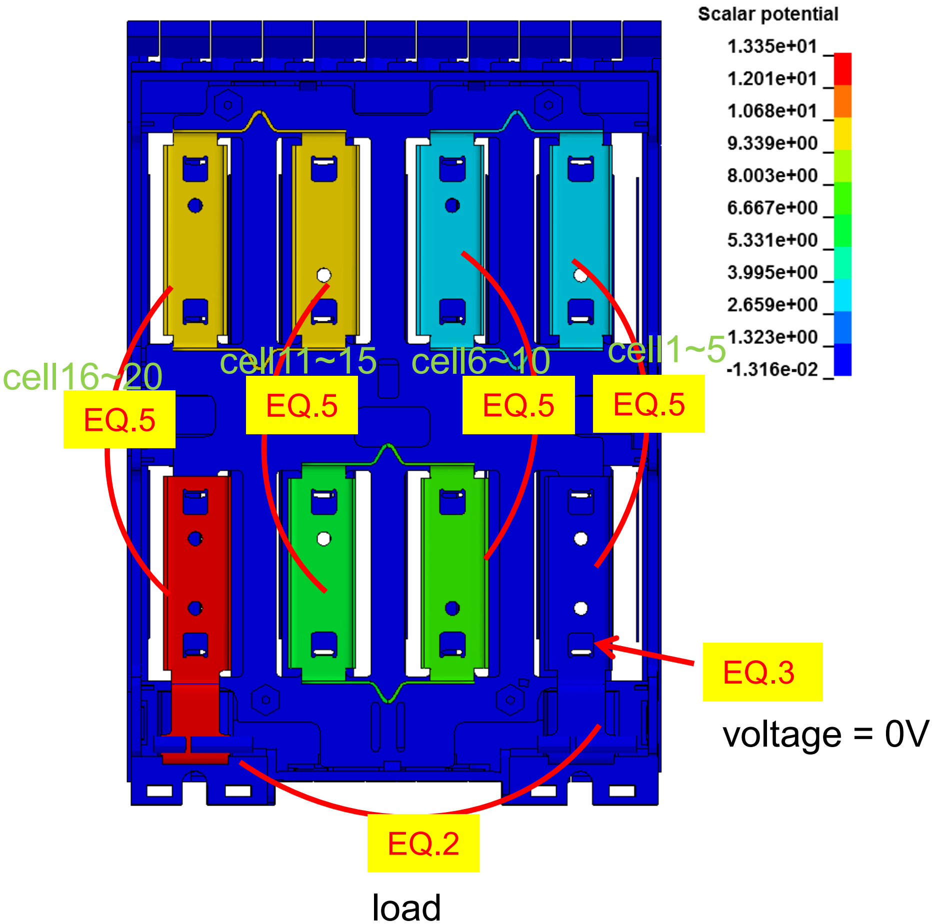


Indenter speed = 1mm/ms

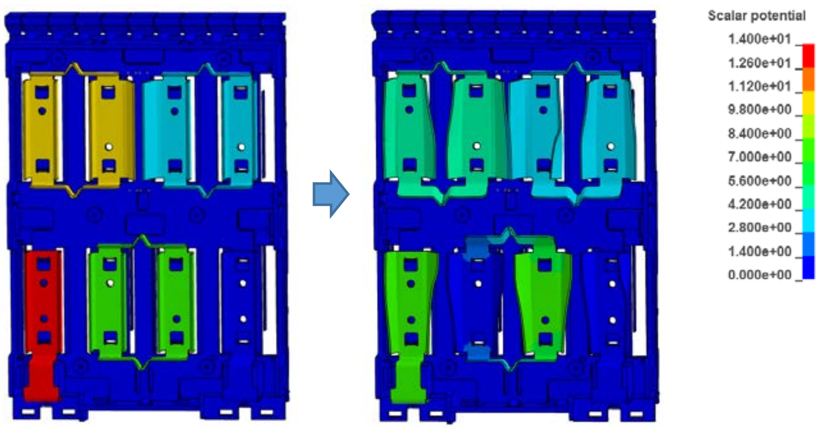
Implementation of Meshless Randle Circuit for External Short - 2.5 s Compression Simulation Results

- Meshless Randle Circuit

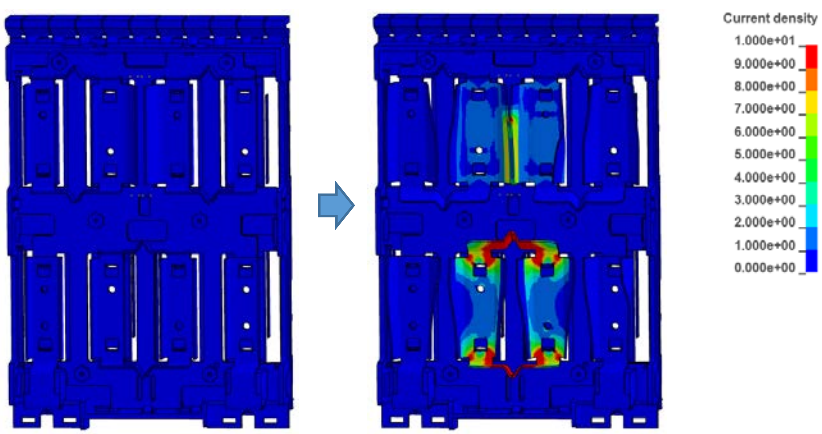
EM connection types:



Electrical Potential



Current Density



Connection Type:
EQ2.: Resistance, EQ.3: Voltage Source, EQ.5: Randle Circuit.

- Electrical potential drop and current density increase shown after external short was captured.

Responses to Previous Year Reviewers' Comments

- A reviewer suggested CT scanning method for the microstructure characterization and visualization of the cell component deformations subject to mechanical loads.
  - A more cost effective method to address this request can be the microstructure model developed based on the SEM images of the cell components (i.e. SEM images of a separator under tensile loads).

Collaboration and Coordination with Other Institutions

- ORNL is developing methods to scale-up detailed mechanical and electrochemical simulations to reduce computational complexity while retaining high fidelity.
  - ORNL also collaborates with Lawrence Berkeley National Laboratory and Sandia National Laboratory under ES295.

- LS-DYNA® is the CAE software of choice for the project and contains key, battery-specific solver enhancements.

Remaining Challenges and Barriers/ Future Research

- Development of the damage and failure models inside the layered solid element.
- Find optimal mechanical models to get correct cell deformations.
- Define the failure condition that triggers internal short circuit.
- Couple the mechanical deformations with the EM models to define the internal short circuit resistances.
- Model development for the larger scale with multiple cells meeting the targeted computational time and memory.

Proposed Future Research

- Carry out characterization tests for the input parameters of the Type-E cell for its model development.
- Develop models for internal short configurations based on the damage and failure in the cells.
- Scale the simulation method to enable durability assessment of modules and packs.
- Development of a battery packaging module in LS-PREPOST to help users set up cases.

Any proposed future work is subject to change based on funding levels.

Summary

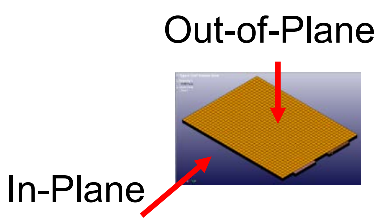
- Layered solid mechanics are being expanded to incorporate battery constitutive models and failure modes.
- Battery-specific solver developments have been incorporated into battery abuse simulation case studies.
- Module-level multiphysics model of crush-to-external short circuit is under development. LSTC has assisted with the de-bugging process and recent results are promising for delivering multiphysics capability with minimal computational cost.
- Methods to represent component mechanics are under development. An optimization approach is being used to build a mesh that replicates an anisotropic separator response.
- Graphical user interface is progressing according to expectations.
- Validation experiments are fully defined and the associated purchase orders were issued.

Technical Back-Up Slides

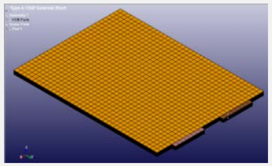
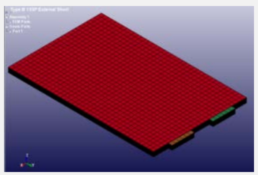
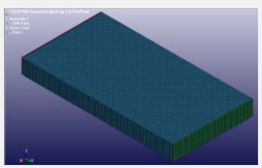
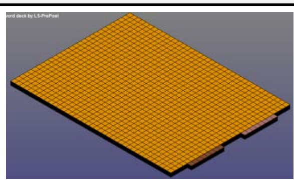
Development Assumptions

	Crash	Regulatory Crush	Overcharge/External Short/Thermal Ramp
Mechanics Time Scale	< 100 ms	> 10 s	> 10 s
EET Time Scale	ms to minutes		
Deformation Mode	Out-of-Plane or In-Plane Compression; Bending; Shear	Out-of-Plane Compression; In-Plane Compression	Internal Swelling; Separator Melting
Solver Assumption	Explicit to Implicit	Implicit	Implicit

- *3-D, transient finite element code needed to span these target applications*
- *Methods to span time scales of mechanics and EET will be developed*

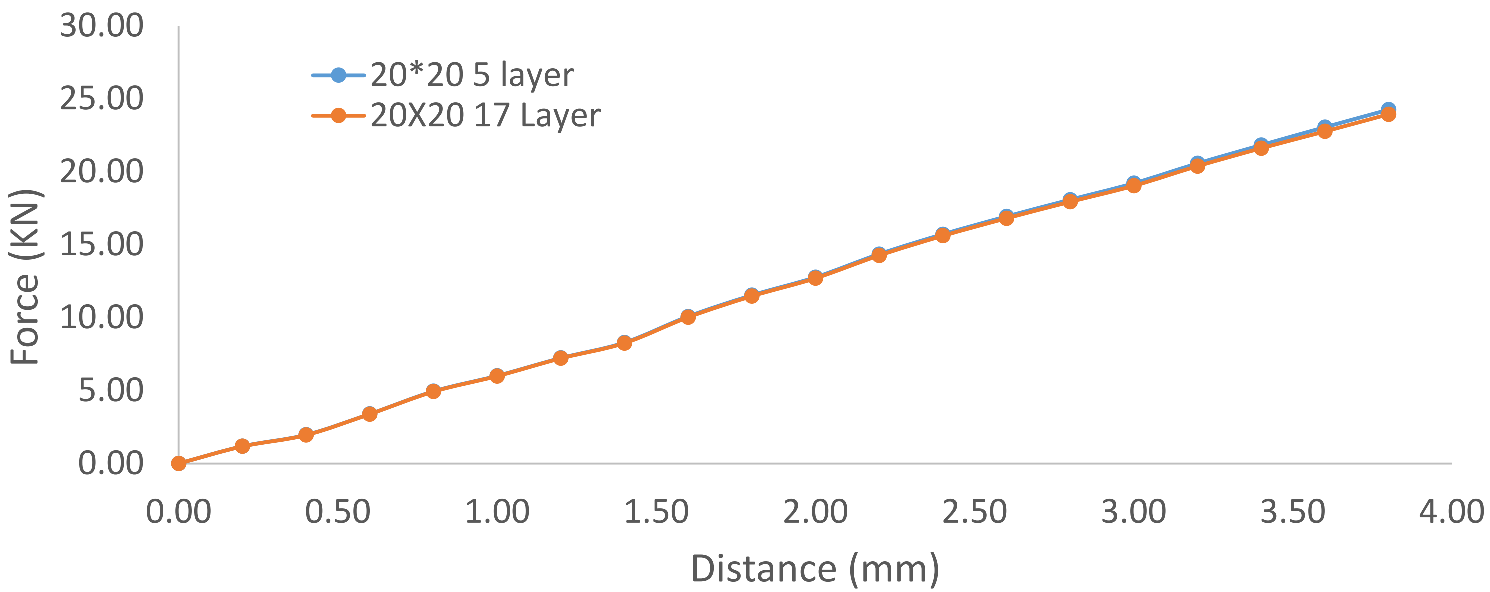


Hardware Selection

Mesh/Geometry	Type	Cathode Chemistry and Format	Cell	Module	Pack
	A	NMC//LMO Blend Pouch	15 Ah 3.7 V 0.06 kWh	4P1S 5P4S	4S5P (x9) + 2S5P (x2)
	B	NMC Pouch	20 Ah 3.6 V 0.07 kWh	3P1S and 3P10S	
	C	LFP Prismatic	18 Ah 3.2 V 0.06 kWh	4P1S 5P2S	36S5P
	D	NMC Pouch	21 Ah 3.65 V	5P4S	4S5P (x9) + 2S5P (x2)
	E	Metal Oxide Blend Prismatic	60 Ah 3.65 V (est)	TBD	

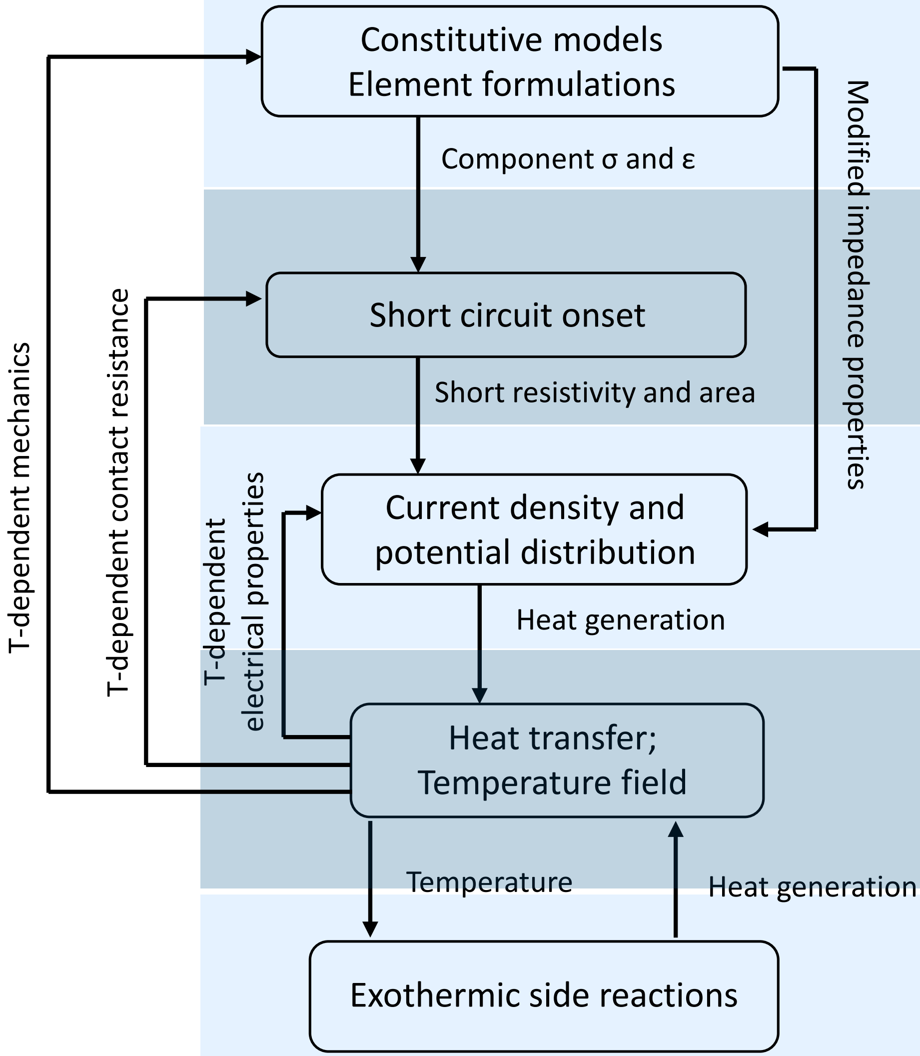
Legacy Hardware ☐ Hardware sourced for this project ☐

Layered Solid Model – Element Discretization and Indentation Simulation Comparison



- Computational time 20X40 17 layers = 632 second
- Computational time 20X20 5 layers = 502 second
- Computation time for solid elements = 52705 second
- Computational time savings = **105** times

Combined Solver Development Assumptions for Crush/External Short Circuit/ Thermal Ramp



*MAT_024
*MAT_063
*MAT_{}

*PART_COMPOSITE
*SECTION
*ELEMENT
*USER_{}

*EM_RANDLE_SHORT
*EM_CONTACT
*EM_ISOPOTENTIAL_CONNECT

*EM_MAT
*EM_CIRCUIT_RANDLE
*EM_ISOPOTENTIAL
*EM_ISOPOTENTIAL_CONNECT

*MAT_THERMAL_{}
*BOUNDARY_CONVECTION_{}
*BOUNDARY_RADIATION_{}

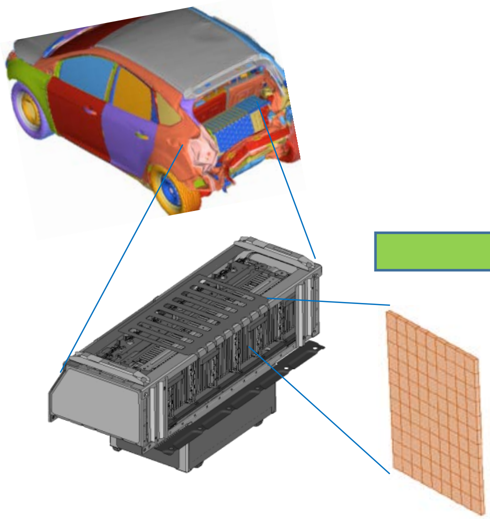
*EM_RANDLE_EXOTHERMIC_REACTION

Virtual Integrated Battery Environment (VIBE)

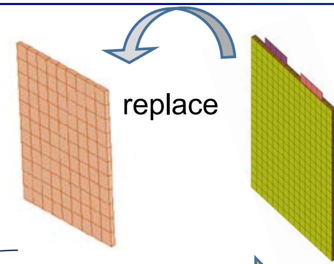
Existing; *New or updated*

Roadmap for Macro, EM Macro, and Meso

Full vehicle CAE with **MACRO** cell model

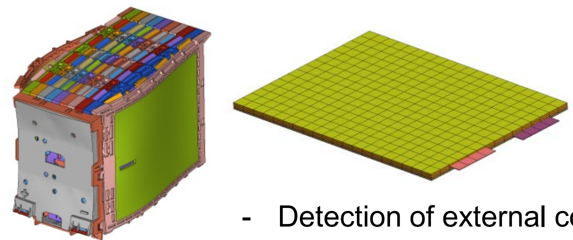


External short circuit flag



External Short

Replace problematic cells with **EM Macro** cells model

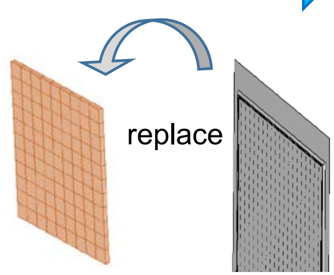


- Detection of external contact
- Subsequent EM and thermal evolution due to external contact

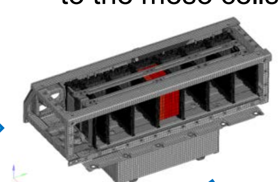
Internal short circuit flag

Replace problematic cells with **MESO** cell models

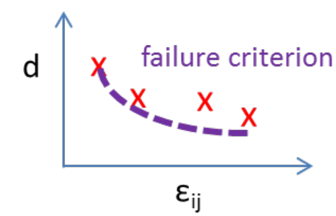
Internal Short



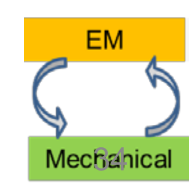
<u>Sub-cycling</u> applied to the meso cells



More accurately identify short circuit using meso cell model failure criteria (smaller safety factor)



Coupled EM/Mechanical response to detect thermal runaway in longer time scale



Model	Cell Elements	Explicit time step
Macro	100-300	7E-4 ms
EM macro	600-2.7k	1E-4 ms
Meso	150k-3.8M	1.6E-6 ms